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DYNAMIC PROGRAMMING AND THE VARIATIONAL SOLUTION OF THE THOMAS—FERMI EQUATION

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SUMMARY

In a recent paper, Ikebe and Kato discussed the use of the variational problem of minimizing $J(u) = \int_0^\infty (u'^2 + \frac{4}{5} u^{5/2} x^{-1/2}) dx$ in connection with the numerical solution of the Emden-Fowler-Thomas-Fermi equation $u'' - u^{3/2} x^{-1/2} = 0$, $u(0) = 1, u(\infty) = 0$.

In this paper, we consider the application of the theory of dynamic programming to this minimization problem and present two approaches. Computational results will be presented subsequently.

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§1. Introduction

In a recent paper, Ikebe and Kato, [8], considered the problem of the numerical integration of the nonlinear equation

$$(1) \qquad u'' - u^{3/2}x^{-1/2} = 0, \quad u(0) = 1, u(\infty) = 0,$$

which arises in connection with the Thomas-Fermi statistical model of a free neutral atom.

The general equation

$$(2) \qquad u'' - u^m x^n = 0, \quad -\infty < m,n < \infty,$$

arose a number of years before in connection with some astrophysical problems, see Emden, [4]. This equation, together with the equations

$$(3) \qquad u'' + u^m x^n = 0, \quad u'' \pm e^{\lambda x} u^n = 0,$$

was discussed in painstaking detail by Fowler in a series of papers, [5], [6], [7], where Emden's results are considerably extended. A unified and in some cases simplified presentation of Fowler's results is contained in the author's book, [3]. A later treatment of these equations is given in Sansone, [9].

In their paper, Ikebe and Kato treat the problem of determining u'(0) by means of the associated variational problem:

Minimize the functional

(4) $$J(u) = \int_0^\infty (u'^2 + \frac{4}{5} u^{5/2} x^{-1/2}) dx$$

over the functions for which the integral exists, and which satisfy tne constraints

(5) $$u(0) = 1, \quad u(\infty) = 0.$$

In this paper, we wish to indicate a new numerical technique for integrating nonlinear differential equations satisfying two-point boundary conditions which arise from variational problems. This is based upon the new approach to the calculus of variations embodied in the theory of dynamic programming, [1], [2].

Detailed computations based upon these results will be presented subsequently. Here we wish to derive an interesting first order nonlinear differential equation associated with the variational problem, derived from the functional equation technique of dynamic programming. A corresponding result may be obtained for the variational problem associated with

(6) $$u'' - e^{\lambda x} u^m = 0.$$

§2. Dynamic Programming and Two-Point Boundary Problems

Consider the nonlinear differential equation

(1) $$u'' + \frac{1}{2} \frac{\partial g(u,x)}{\partial u} = 0,$$

$$u(a) = c, \quad u(b) = c_1,$$

taken to be the Euler equation of the variational problem:

Minimize

(2) $$J(u) = \int_a^b [u'^2 + g(u,x)]dx$$

over all functions $u(x)$ satisfying $u(a) = c$, $u(b) = c_1$.

For fixed upper limit b and boundary value c_1, let us regard the minimum of $J(u)$ as a function of the lower limit a, and the value of $u(a)$, namely c, for the range of values $-\infty < a < b$, $-\infty < c < \infty$

We write

(3) $$f(a,c) = \operatorname*{Min}_u J(u)$$

Then, as we have shown before, [1], [2], the function $f(a,c)$ satisfies the nonlinear partial differential equation

(4) $$-\frac{\partial f}{\partial a} = \operatorname*{Min}_v \left[v^2 + g(c,a) + v\frac{\partial f}{\partial c} \right],$$

which yields

(5) $$\frac{\partial f}{\partial a} = \frac{1}{4} \left(\frac{\partial f}{\partial c} \right)^2 - g(c,a).$$

We must be careful about imposing boundary conditions, since as $a \to b$, assuming that $\int_a^b g(u,x)dx \to 0$, we have

(6) $$f(a,c) \text{ or } \frac{(c-c_1)^2}{(b-a)}.$$

Actually, for numerical purposes, it is better to use a discrete version of the original problem than a finite difference scheme associated with (5), cf. [1]. We shall discuss these matters in a subsequent paper.

The slope $u'(a)$ is equal to the minimizing v in (4), which in this case has the value

(7) $$v = -\frac{1}{2}\frac{\partial f}{\partial c}\ .$$

Thus the determination of the function $f(a,c)$ yields all essential information.

§3. A First Order Differential Equation

Let us now apply the foregoing results to the case where $g(u,x) = u^m x^{-n}$. Consider the function defined by

(1) $$f(a,c) = \operatorname*{Min}_{u} \int_a^\infty \left(u'^2 + \frac{u^m}{x^n}\right) dx,\ u(a) = c,$$

for $a > 0$.

We begin with the following transformations

(2) $$x = ay,\ w(y) = u(ay)a^{-k},$$

yielding

(3) $$f(a,c) = \operatorname*{Min}_{w} \int_1^\infty \left(a^{2k-1} w'^2 + a^{km-n+1}\frac{w^m}{x^n}\right) dx,$$

$$w(1) = c/a^k.$$

Now choose k so that the exponents of a are equal, $2k-1 = km-n+1$, or

(4) $$k = \frac{2-n}{2-m}\ .$$

We assume that $m \neq 2$, i.e. the Euler equation is actually nonlinear. Thus

(5) $$f(a,c) = a^{\frac{2+m-2n}{2-m}} \operatorname*{Min}_{w} \int_1^\infty \left(w'^2 + \frac{w^m}{x^n}\right) dx,$$

$$w(1) = c\ /\ a^{(2-n)/(2-m)}\ .$$

From this we see that $f(a,c)$ satisfies the functional relation

(6) $$f(a,c) = a^{\frac{2+m-2n}{2-m}} f(1, c/a^{(2-n)/(2-m)}).$$

We can then write

(7) $$f(a,c) = a^{\frac{2+m-2n}{2-m}} \phi(c/a^{(2-n)/(2-m)}),$$

with

(8) $$\phi(x) = f(1,x).$$

Let us now apply the partial differential equation of (2.5), which in this case is

(9) $$\frac{\partial f}{\partial a} = \frac{1}{4} \left(\frac{\partial f}{\partial c} \right)^2 - c^m a^{-n}.$$

We have

(10) $$\frac{\partial f}{\partial a} = \left(\frac{2+m-2n}{2-m} \right) a^{\frac{2(m-n)}{(2-m)}} \phi\, (c/a^{(2-n)/(2-m)}) - \left(\frac{2-n}{2-m} \right) ca^{-\left(\frac{2-n}{2-m} + 1 \right)} \phi'(c/a^{(2-n)/(2-m)})\, a^{\frac{2+m-2n}{2-m}},$$

$$\frac{\partial f}{\partial c} = a^{\frac{2+m-2n}{2-m} - \left(\frac{2-n}{2-m} \right)} \phi'(c/a^{(2-n)/(2-m)}).$$

Now set $x = c/a^{(2-n)/(2-m)}$ and substitute in (9). The resultant equation for $\phi(x)$ is

(11) $$\left(\frac{2+m-2n}{2-m} \right) \phi(x) - \left(\frac{2-n}{2-m} \right) x\phi'(x) = \frac{\phi'(x)^2}{4} - x^m.$$

Since $\phi(x) = f(1,x)$, we see that $\phi(o) = o$.

Since this is a singular differential equation, its numerical integration requires some care. Observe that if $f(a,1)$ is continuous in a, (which can be demonstrated), we have

$$\text{(12)} \qquad f(0,1) = \lim_{a \to 0} f(a,1) = \lim_{a \to 0} a^{\frac{2+m-2n}{2-m}} \phi(1/a^{(2-n)/(2-m)})$$

$$= \lim_{x \to \infty} x^{\frac{2n-m-2}{2-n}} \phi(x),$$

provided that $m < 2$, $n < 2$. It is clear that we actually want $n < 1$, in order that the integral in (3.1) exist.

We shall discuss this in detail in a subsequent paper devoted to computational results.

§4. The Equation $u'' - \left(\frac{n+1}{2}\right) e^{\lambda x} u^m = 0$.

In similar fashion, consider the variational problem:

"Minimize

$$\text{(1)} \qquad J(u) = \int_a^{\infty} (u'^2 + e^{\lambda x} u^m)\, dx,$$

over all functions u for which the integral exists and for which $u(a) = c$."

Define

$$\text{(2)} \qquad f(a,c) = \min_u J(u).$$

Then, as above, we obtain the relation

$$\text{(3)} \qquad f(a,c) = e^{\frac{2\lambda a}{2-m}} f(0, ce^{-\frac{\lambda a}{2-m}})$$

$$= e^{\frac{2\lambda a}{2-m}} \phi(ce^{-\frac{\lambda a}{2-m}}).$$

Using the partial differential equation of (2.5), we obtain a first order differential equation for $\phi(x)$ similar to that of (3.11).

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